Development of Algorithms and Strategies for Monitoring Chlorophyll and Primary Productivity in Coastal Ocean, Estuarine and Inland Water Ecosystems

Quarterly Technical Report
January 15, 1997

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Summary

This is the second quarterly progress report for a contract that began in May, 1996, for the Definition Phase of a MODIS Instrument Team investigator project. The Definition Phase contract covers the period from May 13, 1996, through June 30, 1997. The central objective of the Definition Phase contract is:

> To establish a protocol for developing and validating regional or site-specific algorithms for estimating surface chlorophyll-a concentration and primary productivity while accounting for optical variability of other water constituents.

This report describes progress in three areas: (1) chlorophyll algorithm protocol development (2) primary productivity algorithm protocol development and (3) participation in MODIS Science Team meetings and related activities.

Chlorophyll Algorithm Protocol Development

This objective is largely theoretical in nature. The end result will be a paper that describes the general approach to parameterizing and validating the chlorophyll algorithm while accounting for optical variability of other water constituents found in coastal, estuarine and inland waters. There are 5 tasks involved in accomplishing this objective.

The basis for the chlorophyll algorithm will be a radiance model relating upwelling spectral radiance above the water surface, $L_w(\lambda_i)$, to the inherent optical properties of the water, specifically to the backscattering coefficient $b_b(\lambda_i)$, and the absorption coefficient, $a(\lambda_i)$. The inherent optical properties (IOPs) are then related to constituents in the water. Constituents of interest include phytoplankton chlorophyll (CHL), chromophoric dissolved organic matter (CDOM), and total suspended sediments (TSS).

A radiance model, run in the forward direction, predicts spectral radiances given constituent concentrations and other properties of the in-water constituents. The bio-optical algorithm is the inverse of the radiance model. That is, it predicts constituent concentrations and their optical properties given spectral radiances derived from atmospherically corrected satellite observations. Radiance models involving inherent optical properties generally involve their ratio:

$$\frac{b_b(\lambda_i)}{a(\lambda_i) + b_b(\lambda_i)} = \frac{b_b(\lambda_i)/a(\lambda_i)}{1 + b_b(\lambda_i)/a(\lambda_i)} = \frac{b_b(\lambda_i)}{a(\lambda_i)}$$

Progress/discussion to date on each of the tasks is as follows:

1. *Evaluation of several candidate algorithms based on radiance models*

This task has been completed. Considerations were discussed in the first progress report (October 1996). Based on our evaluation, we have also accomplished the second task

2. *Final selection of a radiance model and algorithm*

We have chosen the “semi-analytic” radiance model (SRM) of Gordon et al., (1988) to use as the basis for relating normalized water-leaving radiances to the ratio $X = b_b/a$ (Table 1). However, we have modified the model in that we use the absorption coefficient rather than a K model (as was done by Gordon et al. (1988) to replace $a+b_b$).

Table 1. Equations used to derive L_{wn} from b_b and a (left column) and the inversion equations used to derive b_b/a from L_{wn} (right column). Eqs. 1.1 to 1.3 predict the normalized water-leaving radiance given a and b_b whereas eqns. 1.4 to 1.6 are the basis for analytical algorithms used to derive in-water optical properties gives water-leaving spectal radiance measurements.

Given the inherent optical properties, a and b_b, we define x’ as follows:	Given normalized water-leaving radiance, L_{wn}, equation (1.3) is inverted to obtain the remote-sensing reflectance
$x' \equiv \frac{b_b}{a+b_b}$ (1.1)	$\frac{R}{Q} = \frac{L_{wn}/F_0}{M + rQ^* L_{wn}/F_0}$ (1.4)
where a and b_b are the effective absorption and back-scatter coefficients within the upper optical depth.	where $M = (1-p)(1-p')/m^2$. Note that both L_{wn} and F_0 depend on wavelength, whereas the other terms in (1.4) do not.
Based on results of Gordon (1986), the remote-sensing reflectance is accurately represented as:	**Equation (1.2) is a quadratic equation with two roots. The only positive root is:**
$\frac{R}{Q} = 0.0949\, x + 0.0794\, x'^2$ (1.2)	$x' = \frac{-0.0949 + \sqrt{0.0090 + 0.3176\, R/Q}}{0.1588}$ (1.5)
for solar zenith angles $0_0 > 20°$.	
According to the “Semianalytic Radiance Model” of Gordon et al., (1988), the normalized warn-leaving radiance can be modeled as:	Since $a >> b_b$ in most Case 1 waters, equation (1.1) is often approximated by X'. ~ b_b/a. However, this approximation is unnecessary, since the ratio of b_b to a is easily computed as:
$L_{wn} = \frac{(1-p)(1-p')F_0 R/Q}{m^2(1-rQ^*R/Q)}$ (1.3)	$\frac{b_b}{a} = \frac{X'}{1-X'}$ (1.6)
where Q* is an estimate of Q, and other symbols are defined in the text. The term (1-rR) which appears in Gordon et al. (1988), has been replaced by (1-rQ*R/Q). Q* does not need to be particularly accurate since (1-rR) varies from about 0.92 to 1.0, and is often assumed to be 1.0.	Thus, beginning with normalized water-leaving radiances in k spectral bands of a satellite ocean color sensor, the variables X'_i, i = l,...,k, can be computed, and these used to compute the ratio of backscatter, $b_b(\lambda_i)$, to absorption $a(\lambda_i)$, at the center wavelengths, λ_i, i = 1,...&

The equations in Table 1 clearly show that the relationship between X and L_{wn} is nonlinear. However, within the dynamic range ($0 < L_{wn} < 2.5$ mW cm^{-2} µm^{-1} sr^{-1}) characteristic of most oceanic waters, the relationship is very nearly linear (Fig. 1). The parameters used to derive X from& are listed in Table 2(a).

Table 2. Parameters used in the prototype algorithm and radiance model.

(a) Parameters used to derive X from water-leaving radiance (Table 1). F_o= extraterrestrial solar irradiance (mW cm^{-2} μm^{-1} sr^{-1}); M = (1-p) (l-p')/m^2. Constants used were: p =0.021, m = 1.33, r= 0.48, and Q* =4.

	$F_o(\lambda)$	ρ'		rQ*
443	179.7	0.2885	0.53748	**1.92**
520	182.4	0.02555	0.53931	1.92
550	181.8	0.02471	0.53978	1.92

(b) Parameters of the phytoplankton absorption coefficient model based on Bricaud et al. (1995). The pure seawater absorption, $a_w(\lambda)$, is from Pope (1993).

	$a_w(\lambda)$	$A(\lambda)$	$B(\lambda)$
443	0.0090	0.0393	-0.340
520	0.0474	0.0143	-0.196
550	0.0654	0.0080	-0.052

(c) Parameters of the particle backscatter coefficient model. These $b_{bp}(\lambda)$ model parameters were based on the model of Gordon et al. (1988), where they assumed b^0 = 0.3 m^{-1} and $A_b(\lambda)$ was proportional to b^0. The $A_b(\lambda)$ values given here are normalized to b^0 = 0.3 m^{-1}.

	$b_w(\lambda)$	$A_b(\lambda)$	$B_b(\lambda)$
443	0.00239	0.0100	0.225
520	0.00120	0.0109	0.332
555	0.00095	0.0110	0.358

This approach gives us the flexibility to test sub-component models for the absorption and backscattering by various water constituents. Specifically, we can select from a number of absorption and backscattering coefficient models for phytoplankton chlorophyll, CDOM, TSS, etc. These are then used to calculate the total absorption and backscattering coefficients as the sum of the absorption and backscattering coefficients for all of the components in seawater. In Case 1 waters, the only particles in the water are phytoplankton and their breakdown products such as detritus and CDOM. Case 2 waters will have other constituents such as TSS.

For waters with a single type of particle, the backscattering coefficient is $b_b = b_{bw} + b_{bp}$ where b_{bw} = backscattering coefficient of seawater, and b_{bP} = backscattering coefficient of the particles. The total absorption coefficient is $a = a_w + a_g + a_{th}$ where a_w = absorption coefficient of seawater, a_g = absorption of gelbstoff (yellow matter or CDOM) and detritus, and a_{th} = absorption of phytoplankton.

Spectral values for a_w and b_{bw} have been previously measured. We use a_w values from Pope, unpublished (taken from the Wetlabs AC-9 calibration manual, 1996), and bb_w values from Smith and Baker (198 1).

Available component sub-models that we will be testing in future work

Absorpti on Models

a_g = gelbstoff absorption (dissolved sea salts and dissolved humic acids)

The a_g Model

$$a_g = a_g(\lambda 0) \times e^{(-S(\lambda - \lambda 0))}$$

where

s = 0.0145 (shape factor, range: $0.011 < S < 0.017$)

$a_g(\lambda 0) = a_g(375) \geq 0.06\ m^{-1}$

a_ϕ - phytoplankton absorption

The Power Law a_ϕ Model (Bricaud et al., 1995)

Bricaud et al. (1995)

$$a^*_\phi = A(\lambda) \times C^{-B(\lambda)}$$

where

$A(\lambda)$,$B(\lambda)$ are wavelength-dependent parameters (see Table 2b above)

The above equation is for a^*_ϕ, not a_ϕ. The relationship between the two is $a^*_\phi = a_\phi/C$

The Hyperbolic a Model (Carder et al., 1996)

Carder (1996) - MODIS ATBD #21

$$a_\phi = a0(\lambda) \times \exp[a_1(\lambda) \times \tanh(a_2(\lambda) \times \ln(a_0)(675)/a3((\lambda)))] \times a_0(675)$$

which through mathematical substitution and using reduces to:

$$a_\phi = a_0(\lambda) \times \exp[a_1(\lambda) \times [(a_3' - C)/(a_3' + C)]] \times (61.9)$$

where

a0, a1, a2 and a3 are wavelength dependent constants

The a Hoepffner and Sathyendrenath Model
(Heopffner and Sathyendrenath,1993)

$$a_\phi = a^*(\lambda 0) \times a\_bar(\lambda)C$$

Scattering and Backscattering Models

The Gordon b_{bp} Model

Gordon et al. (1988)

$$b_{bp} = b^0 A' C^{B}$$

where

b^0 - variable

A,B - wavelength-dependent constants

The b_{bp} ***Morel Model***

Morel (1988)

$$b_b(\lambda) = b \times b_b(\lambda)$$

where

$$b = b^0 x \ C^{0.62}$$

$$b_b(\lambda) = 0.002 + 0.02 \times (0.5 + 0.25 \times \log C)(550/\lambda)$$

The b_{bp} Gordon K-Model (the Diffuse Attenuation Coefficient Model)

Gordon (1989, 1994)

$$\mathbf{b_{bp} = (K/1.0395D_0) - a_w - a_\phi - a_g - b_{bw}}$$

where

D = 1.1 (This is a function of solar zenith angle and wavlength with an average value of 1.1 and ranges from 1.019 to 1.346- Gordon (1994)

$K(\lambda) = K_W(\lambda) + X_c(\lambda)\, C^{e(\lambda)}$

$K_w(\lambda)$, Xc (λ), and e (λ) are tabulated in Morel, 1988.

The Mathematical b_{bp} model

$$b_{bp}(\lambda) = b_{bt}(\lambda 0) \times (\lambda 0/\lambda)^{n}$$

where

n = 3.3 Hoge and Lyon, 1996

Tasks that remain to be accomplished are:

3. *Parameterizing the model so as to minimize squared error*
4. *Demonstrating and testing the algorithm using actual satellite and in-situ data*
5. *Completion of a journal article or NASA technical report*

<u>Primary Productivity Algorithm Protocol Development</u>

This objective, which is also theoretical in nature, will result in a second paper that describes the general approach to parametrizing and validating a primary productivity algorithm for coastal, estuarine and inland waters. This objective entails 5 tasks (see Timeline).

1. Evaluation of several candidate algorithms

This task is being accomplished as an activity of NASA's Ocean Primary Productivity Working Group. We are conducting a Primary Productivity Algorithm Round Robin (PPARR) which is now in the second round of tests.

A report on the second round of the PPARR was prepared and distributed to participants. Conclusions from that report are in the form of brief answers to the questions addressed. These were:

1. How do algorithm estimates compare with estimates of daily integral primary productivity based on in-situ measurements?

The top-performing algorithms had RMS errors of 0.67 to 0.78 g $Cm^{-2} d^{-1}$ (0.22 to 0.26 decades of log) relative to in-situ estimates of integral daily primary productivity in a sample of 89 stations with wide geographic coverage. Within the sample used, the mean integral productivity was 1.08 g C $m^{-2} d^{-1}$ but it varied by more than two orders of magnitude. Measures of performance in round two were improved over the results of round one which were based on 25 stations and more limited geographic coverage. Biases are a significant source of error in the algorithms, and three maybe reduced by simple reparameterizations.

2. Do some algorithms perform better in a specific region? If so, have these algorithms been parameterized with data from the region? Do they reflect a better understanding of productivity in that region?

Some algorithms tend to perform better in a particular region compared with other regions. It is unknown whether or not this is because they have been parametrized with data from those regions. If so, they may also reflect a better understanding of productivity in a particular region. When the error analysis was performed on a regional basis, RMS errors ranged from 0.10 to 0.47 g $Cm^{-2}d^{-1}$ (0.07 to 0.20 decades of log) for all regions except the Palmer LTER stations where RMS errors were 1.48 g C $m^{-2} d^{-1}$ (0.37 decades of log).

3. How do algorithms compare with one another?

Several algorithms were highly correlated with one another. The top-performing algorithms had correlation coefficients ranging from 0.79 to 0.97. Systematic differences were seen between algorithms that were both highly correlated, as well as between some that were poorly correlated. This comparison of algorithms suggests that differences in algorithms may be explained (or even eliminated) by slight changes in parameterizations.

4. How does the error in a satellite-derived surface chlorophyll measurement affect primary productivity algorithms?

Simulated errors in the surface chlorophyll concentration (Δ_B) resulted in highly correlated errors in primary productivity (Δ_{IPsat}). However, the errors in productivity did not scale in proportion to the chlorophyll errors, but rather they varied as:

$$\Delta_{IPsat} \sim (\Delta_B)^P$$

where p is an exponent ranging from 0.3 to 0.8. Some algorithms were remarkably insensitive to errors in surface chlorophyll suggesting that chlorophyll plays a minor role.

5. How much improvement can be achieved with better knowledge of:

a. the vertical distribution of chlorophyll, temperature, and light?

All algorithms except one improved with the incorporation of vertical profile information. The profile information (chlorophyll, temperature and light) reduced biases as much as 77% (on average 40-50%), and RMS errors by as much as 50% (average 10-20%).

b. the photo-physiological state of the phytoplankton?

All but three algorithms improved with the incorporation of photo-physiological information. The photo-physiological information (P^b_{opt} and alpha) reduced biases as much as 99% (on average by about 35%), and RMS errors were reduced as much as 50% (average 20-30%). However, three algorithms were unable to incorporate the information correctly, and in these cases, their performance deteriorated severely. Evidently, more work is needed to learn how to interpret these parameters. Some participants did not use the information because they said it was too difficult to interpret.

c. vertical profiles *and* photo-physiological state?

The difficulty in interpreting photo-physiological parameters affected the results in step 3 where both types of information were provided for all stations. Only 6 algorithms were tested with all the information in step 3. Most showed some improvement, but not as much as was expected. For those showing improvement, biases were reduced between 13 and 90%, and RMS errors were reduced between 5 and 53%.

Tasks that remain to be accomplished are:

2. *Selection of an analytical model and algorithm for demonstration purposes*

3. *Parametrizing the algorithm so as to minimize squared error*

4. *Demonstrating and testing the algorithm using actual satellite and in-situ data*

5. *Publication of a journal article or NASA technical report*

<u>Participation in MODIS Science Team meetings and related activities</u>

I attended the MODIS ATBD review in November, and a meeting of the MODIS Oceans Discipline Group (MOCEAN) in January, 1997.

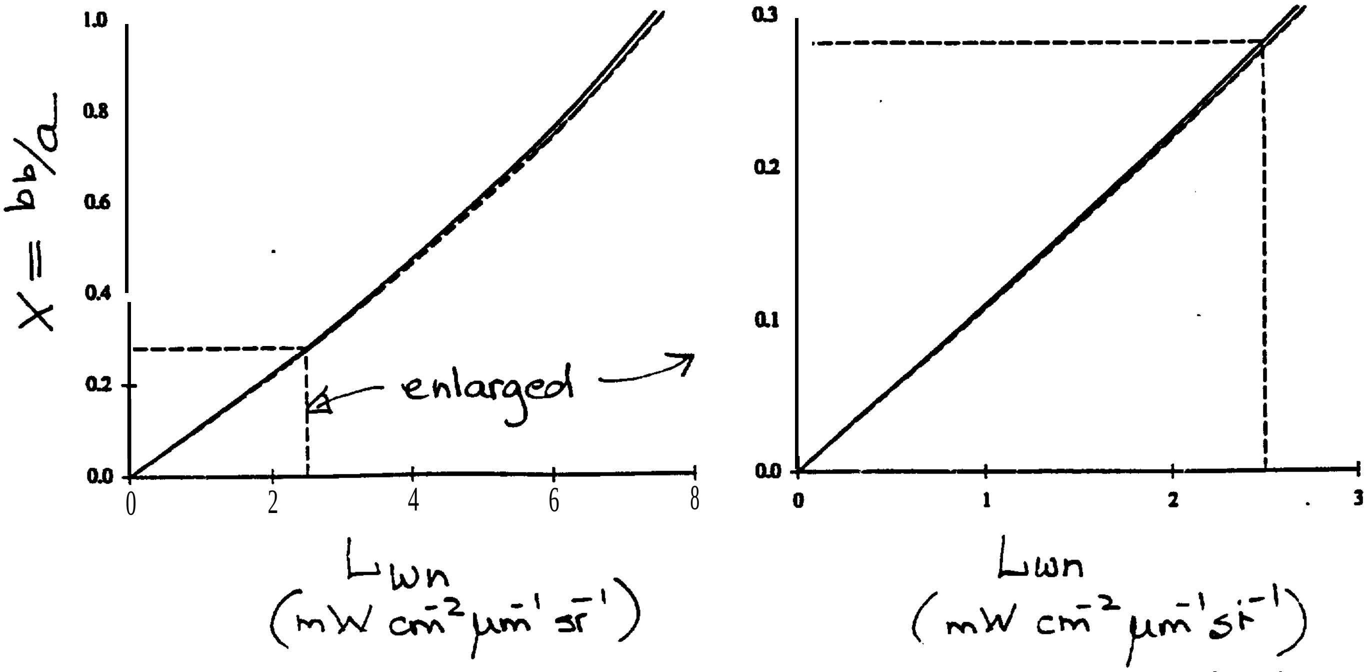

Fig. 1 - Shows relationship (nearly linear) between $X = b_b/a$ and Lwn.